NATIONAL ENERGY TECHNOLOGY LABORATORY

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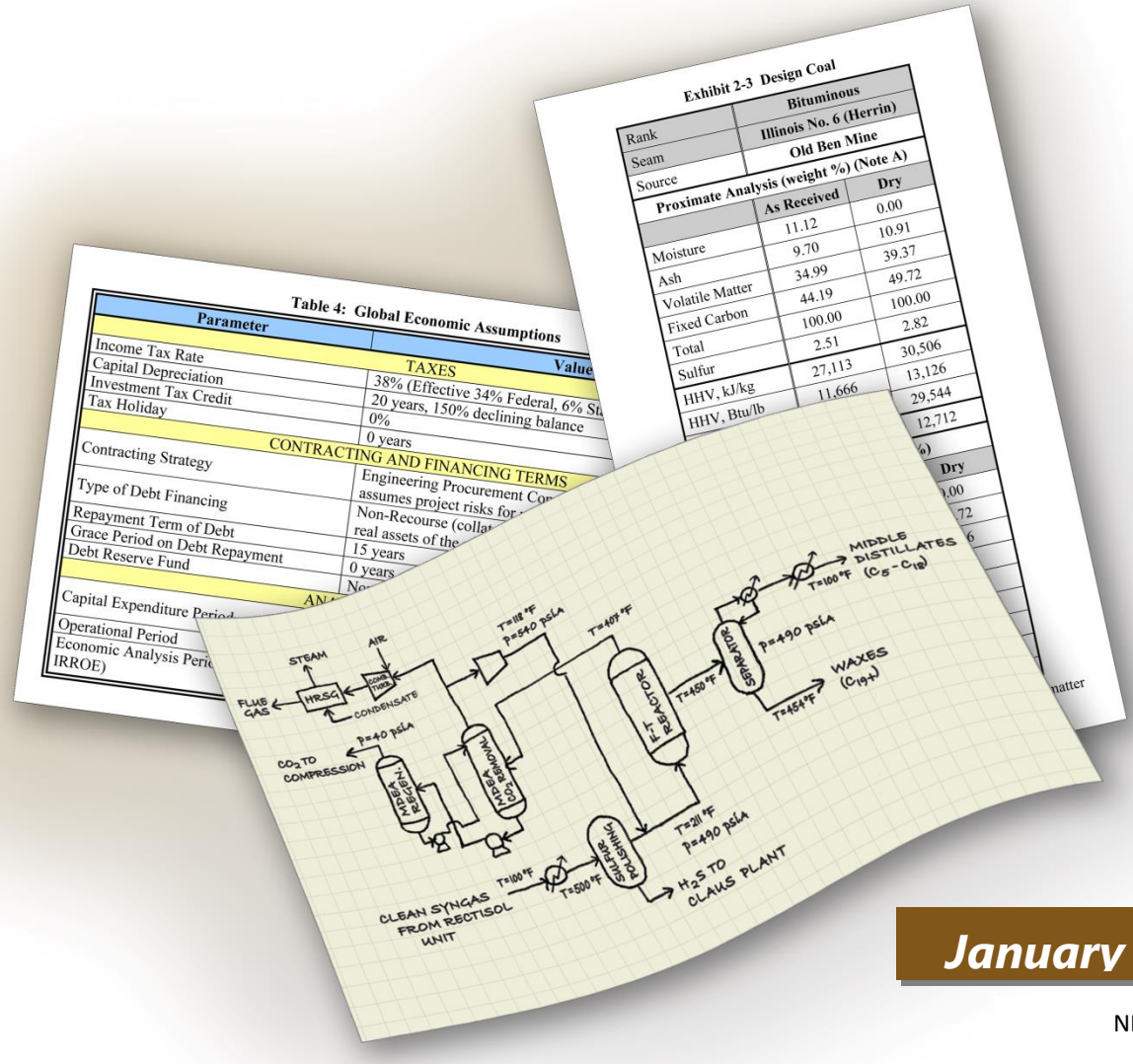
QUALITY GUIDELINES FOR ENERGY SYSTEM STUDIES

Specification for Selected Feedstocks



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Acknowledgments

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List of Exhibits

Acronyms and Abbreviations

CH_4	Methane	H_2	Hydrogen
CO_2	Carbon dioxide	HHV	Higher heating value
DOE	Department of Energy	LHV	Lower heating value
EIA	Energy Information Administration	NETL	National Energy Technology Laboratory
EPA	Environmental Protection Agency	QGESS	Quality Guidelines for Energy System Studies
ESPA	Energy Sector Planning and Analysis	U.S.	United States

1 Specifications for Selected Feedstocks, Products, and Processes

This section provides recommended specifications for various feedstocks that are commonly found in NETL-sponsored energy system studies. Adhering to these specifications should enhance the consistency of such studies. NETL recommends these guidelines be followed in the absence of any compelling market, project, or site-specific requirements in order to facilitate comparison of studies evaluating coal-based technologies.

1.1 Fuel Feedstocks

A short list of commonly used feedstocks is described below. If other fuels are required, they are to be treated with the same rigor of analysis and documentation as the fuels presented below.

1.1.1 Natural Gas

When natural gas is the required fuel, use the composition shown in Exhibit 1-1, which is based on the mean of over 6,800 samples of pipeline quality natural gas taken in 26 major metropolitan areas of the United States (U.S.). [1] Natural gas heating values are the LHV/HHV calculated by Aspen for the natural gas stream, using the natural gas composition listed below.

Exhibit 1-1 Natural gas composition

Component	Volume Percentage	
Methane, CH_4	93.1	
Ethane, C_2H_6	3.2	
Propane, C_3H_8	0.7	
n-Butane, C_4H_{10} [1]	0.4	
Carbon Dioxide, CO_2 [2]	1.0	
Nitrogen, N_2 [2]	1.6	
Methanethiol [3]	$5.75x10^{-6}$	
Total	100.0	
	LHV [4]	**HHV** [4]
MJ/scm	34.52	38.25
kJ/kg	47,201	52,295
Btu/scf	927	1,027
Btu/lb	20,293	22,483

Notes:

1. *The reference data reported the mean volume percentage of higher hydrocarbons (C_4+) to be 0.4%. For simplicity, the above composition represents all the higher hydrocarbons as n-butane (C_4H_{10}).*
2. *The reference data reported the mean volume percentage of CO_2 and N_2 (combined) to be 2.6%. The above composition assumes that the mean volume percentage of CO_2 is 1.0%, with the balance (1.6%) being N_2.*
3. *The sulfur content of natural gas is primarily composed of added mercaptan (methanethiol, CH4S) with trace levels of H2S (11).*
4. *LHV = lower heating value; HHV = higher heating value.*

1.1.2 Coal

Exhibit 1-2 shows ultimate, proximate, and sulfur analyses for eight specific U.S. coals ranging in rank from lignite to low-volatile bituminous. It is recommended that NETL-sponsored studies of coal-fueled systems be based upon one of these coal types and their analyses. Additional information on the coal types (including ash and mineral matter analyses, ash fusion properties, and Hardgrove Grindability Index) is available from the NETL Quality Guidelines section on Detailed Coal Specifications. [2]

Exhibit 1-2 Analysis of selected coals

Rank	Low-Sodium Lignite		High-Sodium Lignite		Sub-bituminous		"Super-compliance" Subbituminous		HV Bituminous		HV Bituminous		MV Bituminous		LV Bituminous	
Seam	Wilcox Group		Beulah-Zap		Montana Rosebud PRB, Area D		Wyodak-Anderson (PRB)		Illinois #6		Pittsburgh #8		Upper Freeport		Pocahontas #3	
Sample Location	TX		Freedom, ND		Montana		Campbell Co. WY						Indiana Co., PA		Buchanan Co., VA	
Proximate Analysis (weight %)																
	AR	Dry	AR	Dry	AR	Dry	AR	Dry	AR	Dry	AR	Dry	AR	Dry	AR	Dry
Moisture	32.00	0	36.08	0	25.77	0	27.42	0	11.12	0	2.63	0	1.13	0	0.65	0
Ash	15.00	22.06	9.86	15.43	8.19	11.04	4.50	6.20	9.70	10.91	9.17	9.42	13.03	13.18	4.74	4.77
Volatile Matter	28.00	41.18	26.52	41.48	30.34	40.87	31.65	43.61	34.99	39.37	35.82	36.79	29.43	29.77	19.14	19.27
Fixed Carbon (BD)	25.00	36.76	27.54	43.09	35.70	48.09	36.43	50.19	44.19	49.72	52.38	53.79	56.41	57.05	75.47	75.96
HHV, kJ/kg	15,243	22,417	15,391	24,254	19,920	26,787	20,469	26,856	27,113	30,506	30,508	31,331	30,971	31,324	34,718	34,946
HHV, Btu/lb	6,554	9,638	6,617	10,427	8,564	11,516	8,800	11,546	11,666	13,126	13,116	13,470	13,315	13,467	14,926	15,024
LHV, kJ/kg	14,601	21,472	14,804	23,335	19,195	25,810	19,738	25,850	26,151	29,444	29,443	30,238	30,108	30,451	33,818	34,040
LHV, Btu/lb	6,277	9,231	6,364	10,032	8,252	11,096	8,486	11,113	11,252	12,712	12,658	13,000	12,944	13,092	14,539	14,635
Ultimate Analysis (Weight %)																
	AR	Dry	AR	Dry	AR	Dry	AR	Dry	AR	Dry	AR	Dry	AR	Dry	AR	Dry
Moisture	32.00	0	36.08	0	25.77	0	27.42	0	11.12	0	2.63	0	1.13	0	0.65	0
Carbon	37.70	55.44	39.55	61.88	50.07	67.45	50.23	69.21	63.75	71.72	73.15	75.13	73.39	74.23	86.15	86.71
Hydrogen	3.00	4.41	2.74	4.29	3.38	4.56	3.41	4.70	4.50	5.06	4.97	5.10	4.03	4.07	4.20	4.23
Nitrogen	0.70	1.03	0.63	0.98	0.71	0.96	0.65	0.89	1.25	1.41	1.46	1.50	1.33	1.35	1.26	1.27
Chlorine	0.02	0.03	0.00	0.00	0.01	0.01	0.02	0.03	0.15	0.17	0.04	0.04	0.00	0.00	0.19	0.19
Sulfur	0.90	1.32	0.63	0.98	0.73	0.98	0.22	0.30	2.51	2.82	2.36	2.42	2.29	2.32	0.66	0.66
Ash	15.00	22.06	9.86	15.43	8.19	11.03	4.50	6.20	9.70	10.91	9.17	9.42	13.03	13.18	4.74	4.77
Oxygen (BD)	10.68	15.71	10.51	16.44	11.14	15.01	13.55	18.67	7.02	7.91	6.22	6.39	4.80	4.85	2.15	2.17
Sulfur Analysis (weight %)																
	AR	Dry	AR	Dry	AR	Dry	AR	Dry	AR	Dry	AR	Dry	AR	Dry	AR	Dry
Pyritic	-	0.43	-	0.34	-	0.63	-	0.07	-	1.14	-	1.47	-	1.77	-	0.15
Sulfate	-	0.04	-	0.09	-	0.01	-	0.01	-	0.22	-	0.05	-	0.01	-	0.03
Organic	-	0.85	-	0.55	-	0.34	-	0.22	-	1.46	-	0.90	-	0.54	-	0.48
Trace Components (ppmd)																
Mercury	-	0.206	-	0.116	-	0.081	-	0.200	-	0.150	-	0.430	-	0.337	-	0.088

Note: AR = as received, PRB = Power River Basin, BD = by difference, HHV = higher Heating Value, LHV = lower heating Value, Refer to [3] for the sources of data except sulfur forms for all lignite, PRB and bituminous HV and chlorine content (Illinois #6) which were extracted from U.S. Geological Survey (USGS) data

1.2 Non-fuel Feedstocks

1.2.1 Limestone

When limestone is required as a feedstock, the analysis in Exhibit 1-3 is recommended for studies that are not site-specific or otherwise require the use of different limestone [4]:

Exhibit 1-3 Greer Limestone analysis

Component	Dry Basis %
Calcium Carbonate, $CaCO_3$	80.40
Magnesium Carbonate, $MgCO_3$	3.50
Silica, SiO_2	10.32
Aluminum Oxide, Al_2O_3	3.16
Iron Oxide, Fe_2O_3	1.24
Sodium Oxide, Na_2O	0.23
Potassium Oxide, K_2O	0.72
Balance	0.43
Total	100.00

1.2.2 Lime

When lime is required as a feedstock, the analysis in Exhibit 1-4 is recommended for studies that are not site-specific or otherwise require the use of different lime. [5]

Exhibit 1-4 Lime analysis

Component	Analysis %
Calcium Oxide, CaO	92.60
Magnesium Oxide, MgO	1.20
Silica, SiO_2	0.95
Aluminum Oxide, Al_2O_3	0.20
Iron Oxide, Fe_2O_3	0.34
Balance	4.71
Total	100.00

2 Revision Control

Exhibit 2-1 Revision table

Revision Number	Revision Date	Description of Change	Comments
1	February 5, 2014	Document formatted	
2	July 20, 2018	Coal compositions for Ill. #6 were changed to be more representative of average compositions rather than for a specific mine. Natural gas heating values were updated to align with Aspen Plus calculations	

3 References

1 Liss, W.H., et al. (1992). *Variability of Natural Gas Composition in Select Major Metropolitan Areas of the United States*. Gas Technology Institute, Vols. GRI-92/0123.

2 U.S. Department of Energy (DOE)/National Energy Technology Laboratory (NETL). (2011). *Quality Guidelines for Energy System Studies, Detailed Coal Specifications.*

3 U.S. Department of Energy (DOE)/National Energy Technology Laboratory (NETL). (2019). *Coal Specifications for Quality Guidelines for Energy System Studies (QGESS).*

4 EPRI/U.S. Department of Energy (DOE). (2000). *Evaluation of Innovative Fossil Fuel Power Plants with CO_2 Removal.* Palo Alto, CA.

5 Graymont. (2011). *Product Specification, High Calcium Quicklime*. formerly Cutler-Magner Company, bought by Graymont in November 2007.